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Atomic-scale model analysis of the feature profile evolution during Si etching in chlorine- and bromine-containing plasmas SHOKI IRIE, YUGO OSANO, MASAHITO MORI, KOJI ERIGUCHI, KOUICHI ONO, Kyoto University — Profile simulations are indispensable for understanding the influences of complex reaction processes in plasma etching, to achieve the nanometer-scale control of etched profiles and critical dimensions. This paper presents an atomic-scale model for the feature profile evolution during Si etching in chlorine- and bromine-containing plasmas. The model incorporated an atomic-scale cellular model of surface reaction layers and the Monte Carlo calculation for the trajectory of ions on feature surfaces, including their reflection on and penetration into surfaces, where the potential function for Cl-Si and Br-Si systems was determined from quantum chemical calculations. The model also took into account the formation of surface reaction layers caused by adsorption of neutrals and penetration of ions, chemical etching, ion-enhanced etching, deposition of etch products and by-products, and surface oxidation. The simulation was performed to reproduce experimental observations in Si etching with Cl_2/O_2 and HBr/O_2 chemistries: profile anomalies near the feature bottom such as footing and microtrenching, sidewall tapering and etched depth depending on feature width, and surface roughness or residues. The mechanisms concerned are discussed in terms of competition between etching and passivation, along with ion reflection on feature surfaces.

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